Multi-phase Chemical Processes Oral Monday 11:30 – 11:50

The Multi-phase Atmospheric Chemistry of Isocyanic Acid, HNCO

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Isocyanic acid is a common and relatively abundant product of combustion of nitrogencontaining fuels, especially biomass. There also appear to be sources of HNCO in the atmosphere from photooxidation of reduced nitrogen species, e.g. amines. Removal of HNCO from the atmosphere by reaction with OH, or other radicals, is very slow (years), and photolysis is less certain but also likely to be slow (months). As a result, wet and dry deposition are the processes controlling atmospheric removal of HNCO. As a weak acid (pKa = 3.7), HNCO exhibits pH-dependent solubility in aqueous solution, and is quite soluble (H>10⁵ M/atm) at physiologic pH (7.4) (e.g. in the human lung). Recent biochemical studies have shown that known smoke-related health effects can be linked to protein carbamylation driven by cyanate ion at solution concentrations (100µM), equivalent to 1 ppbv HNCO in the gas phase. Measurement of HNCO in ambient air by negative ion proton-transfer chemical ionization mass spectrometry has shown that HNCO can often approach or exceed 1 ppbv in plumes from wild or agricultural fires, making it important that we understand potential exposure to this possible health hazard. This presentation will focus on the multi-phase behavior of HNCO and some assessments will be made of the effect of hydrolysis on HNCO atmospheric lifetimes and the importance of aerosolphase reactions to form carbamylated products.

References

(1) Roberts, J. M.; Veres, P. R.; Cochran, A. K.; Warneke, C.; Burling, I. R.; Yokelson, R. J.; Lerner, B. M.; Gilman, J. B.; Kuster, W. C.; Fall, R.; de Gouw, J., *PNAS*, **2011**, *108*, 8966-8971.